LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
Data File : VU048492.D
Acq On : 10 May 2022 15:37
Operator : SY/MD
Sample : N2736-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Title : VOC Analysis

Signal : TIC: VU048492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	96	rBV	139693	152522	14.12%	1.651%
2	1.912	171	178	194	rVB	93045	122055	11.30%	1.321%
3	1.996	198	204	214	rVB2	38311	52421	4.85%	0.567%
4	2.482	345	355	363	rBV4	3223	6800	0.63%	0.074%
5	2.568	370	382	398	rBV	229642	380957	35.28%	4.123%
6	2.678	410	416	419	rBV5	1239	1355	0.13%	0.015%
7	2.797	448	453	460	rVB2	531	718	0.07%	0.008%
8	2.829	460	463	467	rBV2	338	288	0.03%	0.003%
9	2.922	489	492	493	rBV	233	142	0.01%	0.002%
10	2.970	499	507	508	rBV3	1280	1238	0.11%	0.013%
11	3.044	517	530	538	rBV3	17072	37464	3.47%	0.405%
12	3.302	604	610	616	rBV2	203	283	0.03%	0.003%
13	3.363	616	629	644	rVV4	19684	43013	3.98%	0.466%
14	3.420	644	647	649	rBV2	362	193	0.02%	0.002%
15	3.517	675	677	679	rBV	138	99	0.01%	0.001%
16	3.562	689	691	692	rBV	204	64	0.01%	0.001%
17	3.649	716	718	722	rBV	166	127	0.01%	0.001%
18	3.703	729	735	741	rBV5	734	931	0.09%	0.010%
19	3.742	745	747	748	rBV	139	76	0.01%	0.001%
20	3.810	764	768	769	rBV	208	181	0.02%	0.002%
21	3.838	774	777	779	rBV	297	257	0.02%	0.003%
22	3.851	779	781	783	rVB	380	149	0.01%	0.002%
23	3.877	783	789	791	rBV	200	214	0.02%	0.002%
24	3.932	805	806	808	rVB	267	92	0.01%	0.001%
25	3.951	808	812	813	rBV	896	529	0.05%	0.006%
26	4.089	848	855	858	rBV4	958	1316	0.12%	0.014%
27	4.218	893	895	896	rBV4	262	114	0.01%	0.001%
28	4.295	917	919	921	rBV	435	186	0.02%	0.002%
29	4.620	1008	1020	1044	rBV	130601	316471	29.31%	3.425%
30	5.067	1141	1159	1176	rBV	203114	447734	41.46%	4.846%
31	5.240	1209	1213	1221	rVB3	621	768	0.07%	0.008%
32	5.391	1243	1260	1272	rBV3	37811	84687	7.84%	0.917%
33	5.639	1326	1337	1344	rBV5	9539	19673	1.82%	0.213%
34	5.726	1346	1364	1376	rBV2	399286	1079855	100.00%	11.688%
35	5.990	1435	1446	1460	rVB8	9486	21799	2.02%	0.236%
36	6.044	1460	1463	1465	rBV	255	146	0.01%	0.002%

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Title : VOC Analysis

37	6.115	1479	1485	1488	rBV4	735	735	0.07%	0.008%
38	6.250	1513	1527	1558	rBV	347763	659661	61.09%	7.140%
39	6.488	1599	1601	1605	rBV2	329	232	0.02%	0.003%
40	6.552	1607	1621	1622	rBV8	4242	7020	0.65%	0.076%
41	6.604	1636	1637	1643	rVB2	528	406	0.04%	0.004%
42	6.639	1644	1648	1649	rBV	200	159	0.01%	0.002%
43	6.694	1649	1665	1701	rVV	246453	508372	47.08%	5.502%
44	6.819	1701	1704	1706	rBV3	660	317	0.03%	0.003%
45	6.922	1734	1736	1738	rBV	336	109	0.01%	0.001%
46	6.970	1749	1751	1753	rVB	238	74	0.01%	0.001%
47	6.993	1753	1758	1760	rBV3	1410	1291	0.12%	0.014%
48	7.073	1778	1783	1785	rBV3	417	337	0.03%	0.004%
49	7.125	1796	1799	1801	rBV2	185	130	0.01%	0.001%
50	7.160	1802	1810	1812	rBV3	4121	4354	0.40%	0.047%
51	7.292	1848	1851	1853	rBV	379	228	0.02%	0.002%
52	7.330	1861	1863	1865	rVB	197	99	0.01%	0.001%
53	7.395	1875	1883	1891	rBV5	3410	5406	0.50%	0.059%
54	7.488	1908	1912	1915	rVB	580	435	0.04%	0.005%
55	7.504	1915	1917	1919	rBB	119	66	0.01%	0.001%
56	7.520	1919	1922	1924	rBV	265	199	0.02%	0.002%
57	7.565	1924	1936	1950	rBV	105377	199710	18.49%	2.162%
58	7.690	1967	1975	1985	rVB5	4920	9184	0.85%	0.099%
59	7.761	1994	1997	2000	rBV4	977	747	0.07%	0.008%
60	7.899	2028	2040	2056	rVB	494289	836715	77.48%	9.056%
61	8.179	2115	2127	2141	rBV	72514	125616	11.63%	1.360%
62	8.411	2192	2199	2209	rVB3	7685	12254	1.13%	0.133%
63	8.488	2211	2223	2235	rBV3	9474	17305	1.60%	0.187%
64	8.578	2241	2251	2257	rBV	18019	29326	2.72%	0.317%
65	8.632	2257	2268	2288	rBV	408712	713751	66.10%	7.725%
66	8.944	2362	2365	2369	rBV3	397	387	0.04%	0.004%
67	8.993	2377	2380	2382	rVB2	234	137	0.01%	0.001%
68	9.015	2384	2387	2389	rBV	245	142	0.01%	0.002%
69	9.028	2389	2391	2396	rBV2	266	212	0.02%	0.002%
70	9.144	2424	2427	2430	rBV3	485	438	0.04%	0.005%
71	9.198	2433	2444	2455	rVB9	4918	8576	0.79%	0.093%
72	9.269	2455	2466	2476	rBV3	5187	8609	0.80%	0.093%
73	9.327	2476	2484	2499	rBV6	10896	19086	1.77%	0.207%
74	9.417	2499	2512	2531	rBV	490692	824607	76.36%	8.925%
75	9.600	2566	2569	2570	rBV2	1188	629	0.06%	0.007%
76	9.687	2589	2596	2605	rBV6	3720	5769	0.53%	0.062%

LSC Area Percent Report

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Operator : SY/MD
Sample : N2736-13
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Title : VOC Analysis

77	9.880	2649	2656	2663	rBV5	3918	5241	0.49%	0.057%
78	10.073	2713	2716	2719	rBV3	786	577	0.05%	0.006%
79	10.137	2734	2736	2739	rVB2	238	136	0.01%	0.001%
80	10.166	2740	2745	2748	rBV2	649	621	0.06%	0.007%
81	10.185	2749	2751	2753	rVV3	469	154	0.01%	0.002%
82	10.266	2771	2776	2778	rBV3	982	896	0.08%	0.010%
83	10.362	2792	2806	2822	rBV2	56725	104031	9.63%	1.126%
84	10.546	2856	2863	2872	rVB7	3447	5670	0.53%	0.061%
85	10.755	2909	2928	2943	rBV	376544	617866	57.22%	6.688%
86	11.066	3017	3025	3034	rBV8	7816	11615	1.08%	0.126%
87	11.224	3072	3074	3075	rBV	438	147	0.01%	0.002%
88	11.391	3121	3126	3130	rBV7	1983	2718	0.25%	0.029%
89	11.520	3158	3166	3172	rBV5	2294	3289	0.30%	0.036%
90	11.745	3226	3236	3244	rBV7	4208	6977	0.65%	0.076%
91	11.812	3244	3257	3276	rVV	535050	857375	79.40%	9.280%
92	12.009	3311	3318	3323	rBV3	1622	2273	0.21%	0.025%
93	12.192	3364	3375	3395	rVB	515874	838378	77.64%	9.074%
94	12.568	3489	3492	3495	rBV2	432	267	0.02%	0.003%
95	12.607	3502	3504	3508	rBV3	527	398	0.04%	0.004%
96	13.208	3685	3691	3693	rBV4	919	867	0.08%	0.009%
97	13.266	3707	3709	3713	rBV	575	365	0.03%	0.004%
98	13.385	3743	3746	3748	rBV2	714	614	0.06%	0.007%
99	13.491	3776	3779	3780	rBV2	335	191	0.02%	0.002%
100	15.285	4334	4337	4340	rBV3	674	607	0.06%	0.007%

Sum of corrected areas: 9239020

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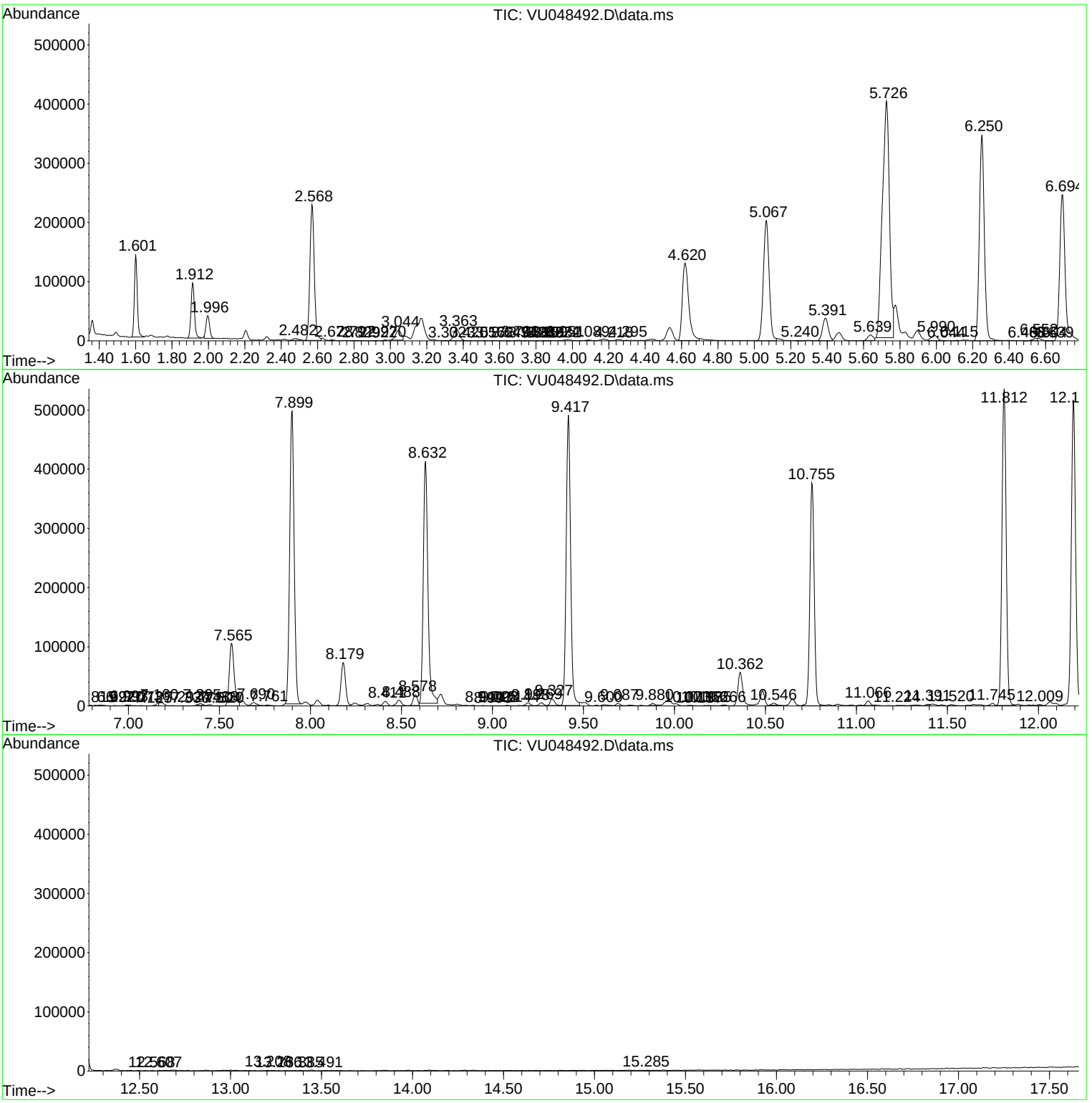
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
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Instrument :
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ClientSampleId :
EXEW9

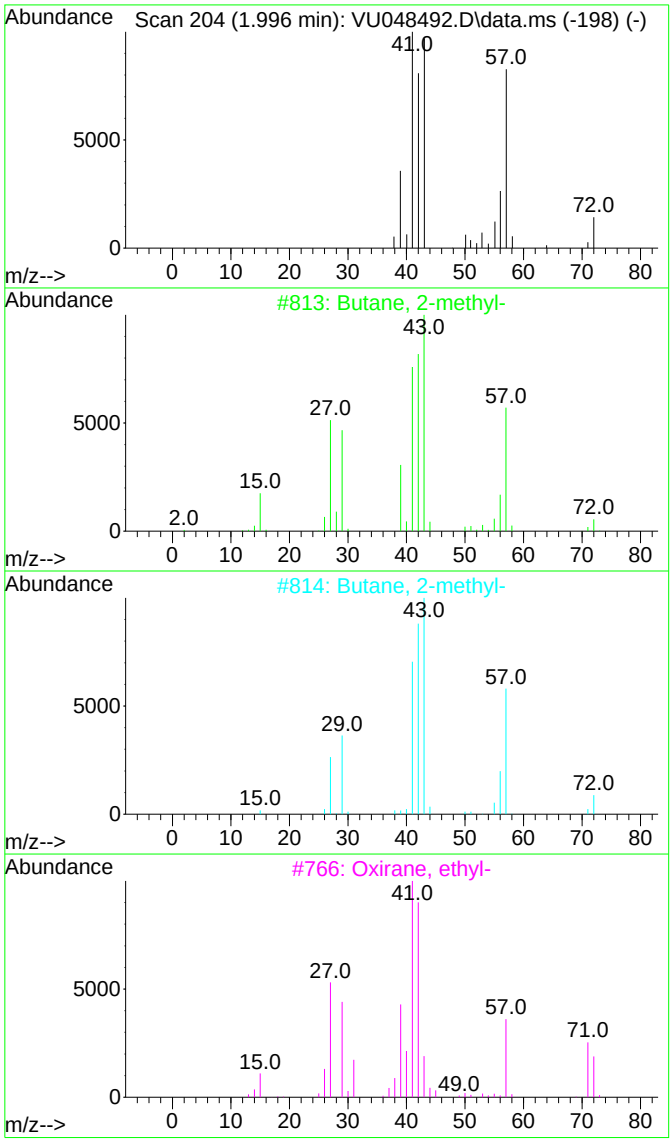
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

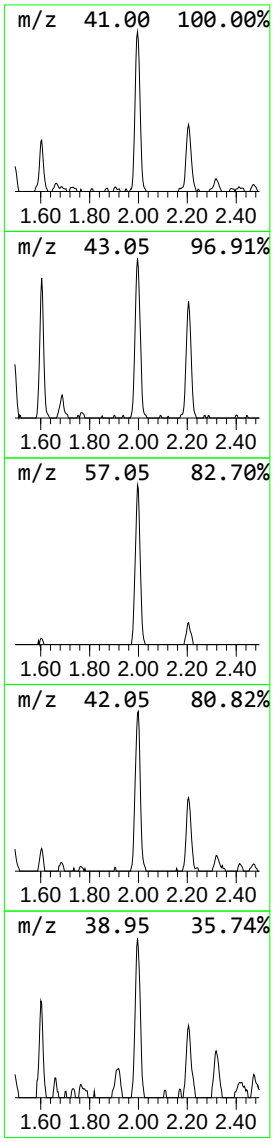
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.996	3.97 ug/L	52421	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	72
2	Butane, 2-methyl-	72	C5H12	000078-78-4	50
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	38
4	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

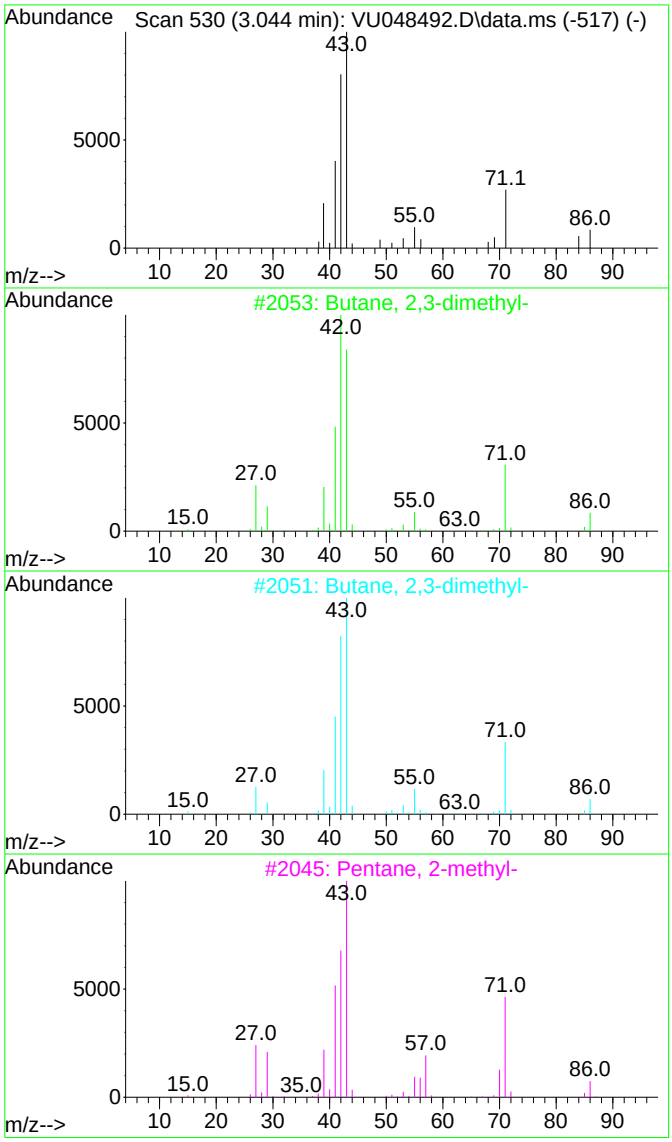
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

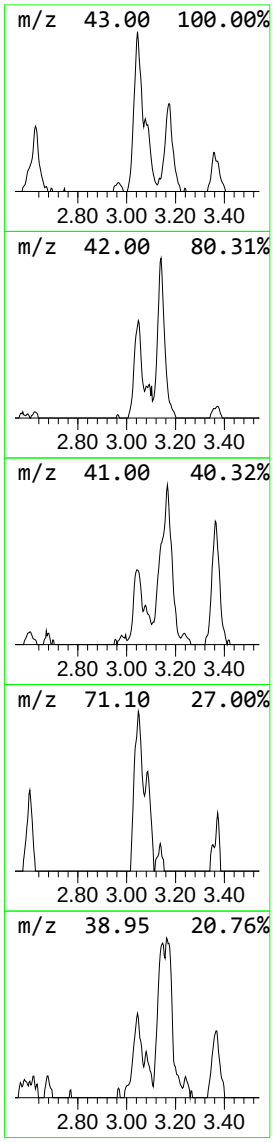
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.044	2.84 ug/L	37464	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	45
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	40
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	12
5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9





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Instrument :
MSVOA_U
ClientSampleId :
EXEW9

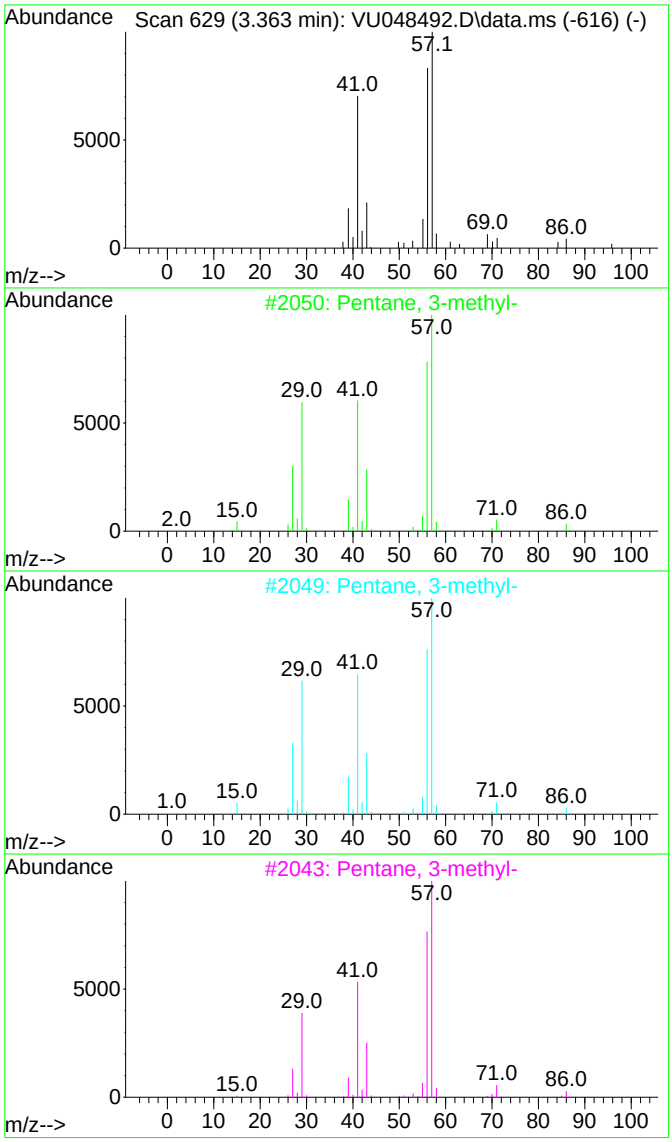
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

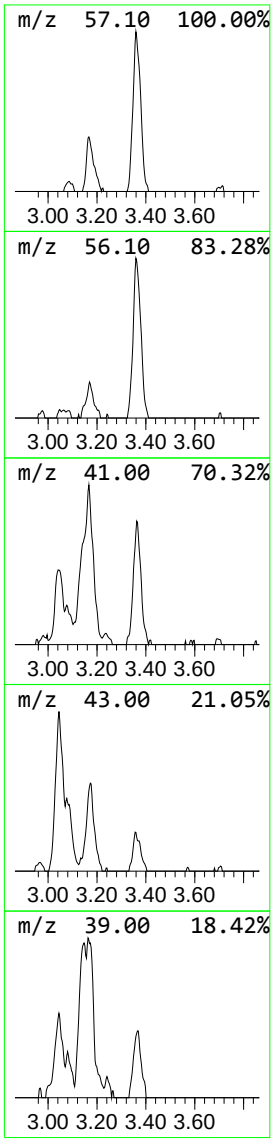
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.363	3.26 ug/L	43013	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2	Pentane, 3-methyl-	86	C6H14	000096-14-0	86
3	Pentane, 3-methyl-	86	C6H14	000096-14-0	72
4	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	56
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56





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Operator : SY/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

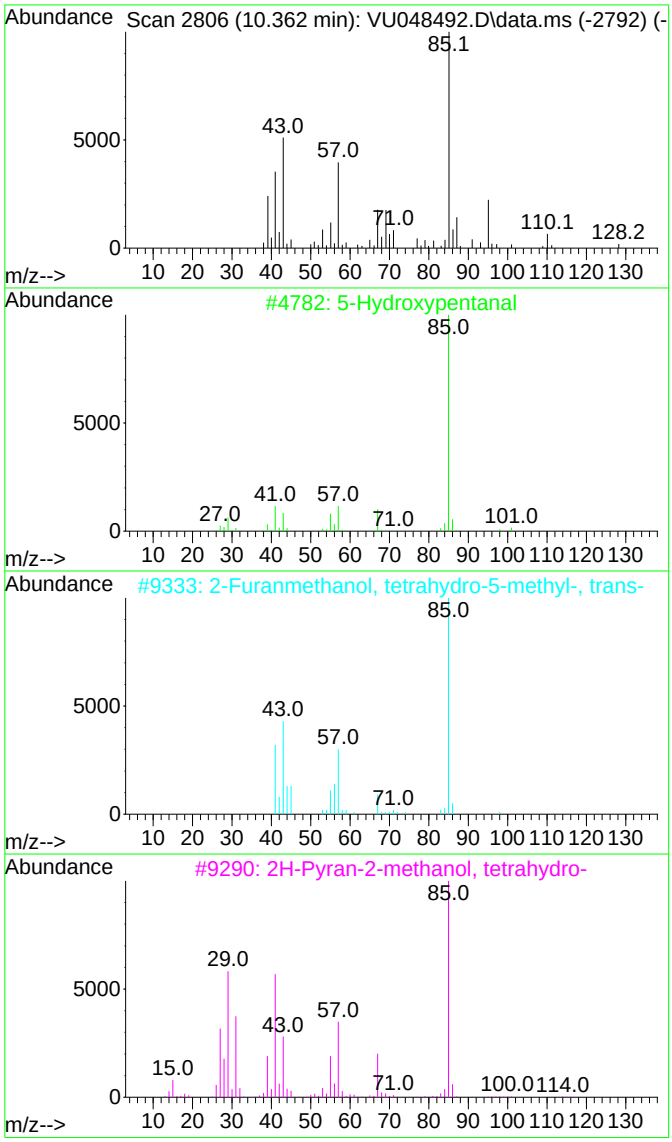
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

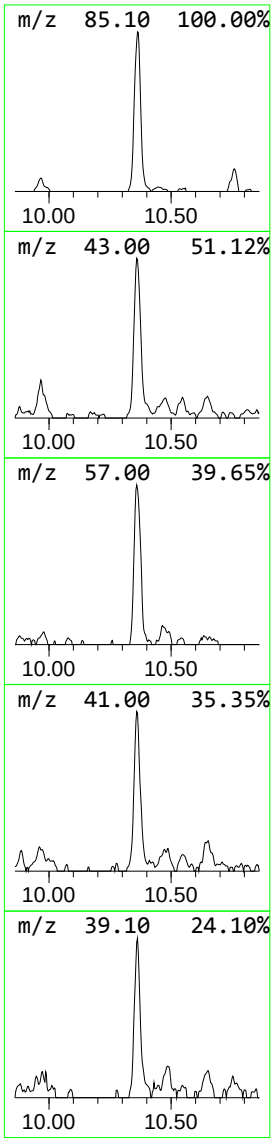
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 5-Hydroxypentanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.362	6.31 ug/L	104031	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Hydroxypentanal	102	C5H10O2	004221-03-8	53
2	2-Furanmethanol, tetrahydro-5-me...	116	C6H12O2	054774-28-6	53
3	2H-Pyran-2-methanol, tetrahydro-	116	C6H12O2	000100-72-1	53
4	1,5-Heptadien-4-ol, 3,3,6-trimet...	154	C10H18O	027644-04-8	53
5	2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	52





Tentatively Identified Compound (LSC) summary

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Data File : VU048492.D
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXEW9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.996	4.0	ug/L	52421	1	6.250	659661	50.0
(DEL) Alkane: S...	3.044	2.8	ug/L	37464	1	6.250	659661	50.0
(DEL) Alkane: S...	3.363	3.3	ug/L	43013	1	6.250	659661	50.0
5-Hydroxypentanal	10.362	6.3	ug/L	104031	2	9.417	824607	50.0